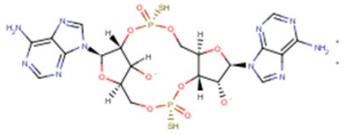
Data Sheet (Cat.No.T10252)

TargetMol
A DRUG SCREENING EXPERT

ADU-S100 disodium salt

Chemical Properties



CAS No.:	1638750-95-4
Formula:	C20H22N10Na2O10P2S2
Molecular Weight:	734.51
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	ADU-S100 (MIW815) disodium salt is an activator of stimulator of interferon genes (STING).
Targets(IC_{50})	STING: None
In vitro	ADU-S100 shows enhanced type I IFN production over CDA in THP-1 human monocytes. ADU-S100 induces the highest expression of IFN-β and the pro-inflammatory cytokines TNF-α, IL-6, and MCP-1 on a molar equivalent basis, as compared to endogenous ML cGAMP and the TLR3 agonist poly I:C. ADU-S100 is also found to induce aggregation of STING and induce phosphorylation of TBK1 and IRF3 in mouse bone marrow macrophage (BMM). ADU-S100 induces significantly higher levels of IFN-α when compared to ML cGAMP.
In vivo	ADU-S100 shows higher anti-tumor control than the endogenous ML cGAMP. A dose-response of the ADU-S100 compound is performed in B16 tumor-bearing mice, which identifies an optimal antitumor dose level that also elicits maximum tumor antigen-specific CD8+ T cell responses, and improves long-term survival to 50%.
Cell Research	Cryopreserved hPBMCs are thawed and 1×10^6 cells per well are plated in a 96 well plate in RPMI media supplemented with 10% FBS, 1% non-essential amino acids, 1% penicillin/streptomycin, L-glutamine, 10 mM HEPES buffer, 1 mM Sodium Pyruvate, 0.055 mM β-ME at 37°C with 5% CO2. Cells are stimulated with 10 μM ADU-S100 or ML cGAMP for 6 hours and supernatants are harvested. Supernatants are diluted 1:2 and assayed for IFN-α protein using Cytometric Bead Array (CBA) Human Flex Set. Data is collected using a FACSVerse cytometer.
Animal Research	WT C57BL/6 mice are inoculated with 5×10^4 B16.F10 cells in the left flank (n=8). When tumor volumes are 100 mm3 mice receive three IT doses of either ML RR-S2 CDG (25 μg), ADU-S100 (50 μg), or HBSS as control. WT C57BL/6 mice are inoculated with 5×10^4 B16.F10 cells in the left flank (n=5). When tumor volumes are 100 mm3 they received three IT doses of ADU-S100 at 5, 25, 50, or 100 μg or HBSS as control. WT C57BL/6 mice are inoculated with 5×104 B16.F10 cells in the left flank (n=8). When tumor volumes are 100 mm3 they receive three IT doses of 100 μg ADU-S100 or HBSS as control. Treatments are administered on days 13, 17, and 20 and tumor measurements are taken twice weekly. Results are shown as percent survival by Log-rank (Mantel-Cox) test (A and C).

Solubility Information

Solubility	H2O: 300 mg/mL (408.44 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.361 mL	6.807 mL	13.615 mL
5 mM	0.272 mL	1.361 mL	2.723 mL
10 mM	0.136 mL	0.681 mL	1.361 mL
50 mM	0.027 mL	0.136 mL	0.272 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Corrales L, et al. Direct Activation of STING in the Tumor Microenvironment Leads to Potent and Systemic Tumor Regression and Immunity. Cell Rep. 2015 May 19;11(7):1018-30.

Tel:781-999-4286 E-mail:info@targetmol.com Address:36 Washington Street,Wellesley Hills,MA 02481